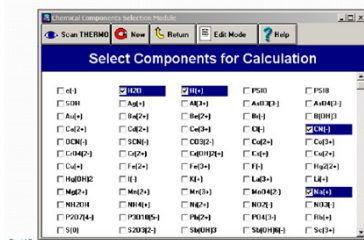


Example 1a (V 4.6)

- Determine the complete species composition from the addition of 5×10^{-3} moles of NaCN to 1 liter of water.
- When you launch MINEQL, it should go right to the "select components" screen
 - If it doesn't, you can get there by selecting: Model>Select components
- This screen contains the Type-I components, which can be selected by clicking on the check-boxes. The components, H_2O and $H(+)$ and already selected for you.
- For this problem, you should then add $CN(-)$ and $Na(+)$.
- Note that $OH(-)$ is not a selection, because it can be obtained by taking an $H(+)$ away from H_2O so that it is not an independent substance. The same is true for HCN (it can be obtained by combining $CN(-)$ and $H(+)$).

Select Components



Example 1b (V 4.6)

- To move on to the Type-II species and the thermodynamic database, hit the "Scan Thermo" button
- This will show the additional species that will form, along with equilibrium constants needed to calculate their concentrations.
- This screen is also the place where you tell MINEQL how much of each component you're adding
- Now move the cursor over to the total concentration line. Keep H_2O and $H(+)$ at zero, but type in 3×10^{-3} for the concentration of $CN(-)$ and the same for $Na(+)$.
- Hit the close button to move on to the next screen
- Select the "Fixed Solids" (i.e., Type-III species). Place the cursor on the pH line and hit the "move" button. Select "move to species not considered (or included)". These are "Type-VI" species. This is necessary, because we don't want to force the pH to stay at any particular level. In fact, one of the purposes of this problem is to determine what the final pH will be.
- You can also do this with the "Wizard"

Figure 1: Screenshot of the 'Type II - Aqueous Species' window in MINEQL+. The window displays a table of species data and a 'Total Conc. [M] -->' section at the bottom.

Name	H2O	H(+)	CN(-)	Na(+)	Log K	Delta H
OH- (-1)	1	1	0	0	-12.997	12.329
HCN (aq)	0	1	1	0	9.210	-10.428

Total Conc. [M] -->

0.000E+00	0.000E+00	5.000E-03	5.000E-05
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Example 1c (V 4.6)

- Hit "close" and then "no" to arrive at the "run time manager"
- Type in an output data name
- Keep "ionic strength corrections", "temperature corrections" and "adsorption model" off
- Hit the "Run" button
- Select "output manager" to view model results
- Header gives input data
- Component Groups has concentrations in a convenient tabular form

Example 1d (V 4.6)

- After the run is complete (should only take a second or two), select "output manager". Under "MINEQL object" select your output file name. Under "member" select "Si.H(+)". Then under "row type" select "species" and under "display criteria" choose "run". This will display the concentrations of all species containing an exchangeable proton (i.e., H+). Copy down the relevant information. Ignore the line labeled "pH". Repeat this process, but this time choose "Si.CN(-)" under the "member" category. This time you will see data on all species that contain the cyanide group (i.e., CN).

Figure 2: Screenshot of the 'Output Manager' window in MINEQL+. The window displays settings for output type, data object, directory, and how to display H(+) data.

Component: H(+)

Output Type: ☐ Header ☐ Log ☐ MultiRun Variables ☒ Component Groups ☐ Special Reports

Data Object: run-01.mdo

Directory: D:_Output

How to Display H(+) Data: ☐ Obs x Variables ☒ Species x Variables ☐ Obs x Species

Variables: [H(+)]

Species: Run 1

Obs: 1. Conc [M]

Buttons: View, Graph IT, Close, Copy, Delete, Help

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- Output Type: Component Groups
- Data Object: CN(-)

run-1m.mdo for CN(-):Run 1

	OBS	SPECIESID	NAME	ITYPE	CONC	LOGC
1	1	20	CH(-)	1	0.00472	-2.33
2	1	30400	HCN (aq)	1	0.000876	-2.56
3	1	224100	NaCN (cubic)	5		-0.23
4	1	600048	TOTAL CH(-)	7	0.005	-2.3

- Output Type: Component Groups
- Data Object: Na(+)

run-1m.mdo for Na(+):Run 1

	OBS	SPECIESID	NAME	ITYPE	CONC	LOGC
1	1	45	Na(+)	1	Se-5	-6.3
2	1	224100	NaCN (cubic)	5		-0.23
3	1	600048	TOTAL Na(+)	7	Se-5	-4.9

Output Manager

Component: Na(+)

Output Type:

- ☐ Header
- ☐ Log
- ☐ MultiRun Variables
- ☐ Component Groups
- ☒ Special Reports

Data Object: run-1m.mdo

Directory: D:_Output

Special Reports

Report Type: Summary of All Species for a Single Run

Run 1

☒ Include Explanation

OK Cancel Help

Input data summary

Summary of All Species for a Single Run

MINEQL+ Ver 4.6

Data Extracted from : run-1m.mdo

SINGLE RUN SUMMARY

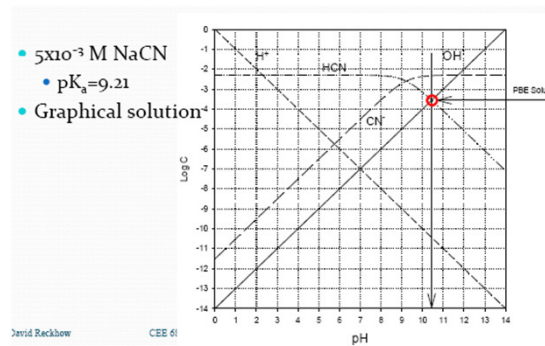
This report compiles the output data (concentration, Log C, Log K) for all species within a single run.

MINEQL+ Ver 4.6

Data Extracted from : run-1m.mdo

Run: 1

ID	Species	Conc.	Log C	Log K
Type I - COMPONENTS				
2 H2O		1.000E+00	0.000	0.000
3 H(+)		3.630E-11	-10.441	0.000
20 CH(-)		4.710E-09	-8.226	0.000
45 Na(+)		6.000E-05	-4.301	0.000
Type II - COMPLEXES				
3800 OH-	(-1)	2.780E-04	-3.556	-14.000
30400 HCN (aq)		2.780E-04	-3.556	9.210
Type III - FIXED ENTITIES				
3901 H2O (solid)				0.000
Type V - DISSOLVED SOLIDS				
224100 NaCN (cubic)			-0.220	-1.600
Type VI - SPECIES NOT CONSIDERED				
175210 pH	(+1)	3.630E-04	-3.441	7.000
Other Species				
900003	Activity of H+	3.630E-11	-10.441	0.000



MINEQL procedure to make Solubility Diagrams

- Select components – Fe³⁺, H⁺, H₂O
- Wizard – put in arbitrary C_T – any value will do
- Fix pH by checking “pH is supplied by user”
- Solids mover – turn all solids off except the one desired
- Close Wizard, view *dissolved solids*, move solid to fixed species
- Run Manager – give file name, specify ionic strength, temperature
- Select MultiRun, titration,
- Select Variable: type of variable = logK, select log K of pH
- Fill in the variable range, # points desired
- Run
- Output Mgr – select file, GraphIt
- Select Component (Fe³⁺), units (logC), species
- Can select only TotalFe³⁺